

Computer-Aided Design of Materials for use under High Temperature

Operating Conditions

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The procedures now in place for producing materials in order to optimize their performance with respect to creep characteristics, oxidation resistance, elevation of melting point, thermal and electrical conductivity and other thermal and electrical properties are essentially trial and error experimentation that tend to be tremendously time consuming and expensive. A computational approach that can replace the trial and error procedures in order that one can efficiently design and engineer materials based on the application in question can lead to enhanced performance of the material, significant decrease in costs and cut down the time necessary to produce such materials. One important application with the possibility of tremendous savings is the development of turbine blades, as it impacts on a variety of applications: power generation and aircraft engines

In order to put into place such a computational methodology one first has to have in hand a robust thermodynamic framework that can describe the response of the class of materials that are being fashioned. One could incorporate the variety of microstructural features such as the dislocation density, lattice mismatch, stacking faults, volume fractions of inclusions, interfacial area, etc., and develop a model and then study its response by solving typical initial-boundary value problems. If the desired response characteristics are known, we can then iterate on the different constituents that go into

making the material until we arrive at the correct mixture that leads to the desired material response. **This is a typical inverse problem wherein we determine the material whose response will meet certain desired characteristics.**

The investigators have already developed a general thermodynamic framework and studied the response characteristics of single crystal superalloys within it. They have developed a detailed computational scheme for studying the response of materials in which the constituents/microstructures can be varied. The computational scheme consists in the development of a user subroutine UMAT (user defined material) in commercial finite element software ABAQUS. In the proposed research, the investigators will develop an interactive optimization scheme whereby models can be systematically varied and their efficacy tested with respect to a desired response. The optimization procedure will be used to design and develop materials so that they can meet the demands of specific problems.